

9-Aza-10-boradecalin

Other names:	Octahydro[1,2]azaborinino[1,2-a][1,2]azaborinine 9-Aza-10-boradecalin
Inchi:	InChI=1S/C8H16BN/c1-3-7-10-8-4-2-6-9(10)5-1/h1-8H2
InchiKey:	VBTBGTSTOFJXPD-UHFFFAOYSA-N
Formula:	C8H16BN
SMILES:	C1CCN2CCCCB2C1
Mol. weight [g/mol]:	137.04

Physical Properties

Property code	Value	Unit	Source
ie	8.47	eV	NIST Webbook
logp	1.867		Crippen Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.50 ± 1.50	K	3.60	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18903543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
tbrp:	Boiling point at reduced pressure

Latest version available from:

<https://www.chemeo.com/cid/64-738-2/9-Aza-10-boradecalin.pdf>

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